

## FINAL TECHNICAL REPORT NASA GRANT NSG-7505

During the last years most of our research was centered on the study of various aspects of the behavior of ices in the solar system and in comets in particular. Connected with it were studies of the outer limits of the solar system, i.e., of the boundary between the Sun-controlled and the Galaxy-controlled motion of cometary nuclei or of other passing small bodies. Out of the latter studies grew our interest in the whole problem of the influence of the galaxy on the solar system. This interest resulted in organization jointly with J.N. Bahcall and M.S. Matthews, and co-sponsored by NASA and by NSF in 1985 in Tucson, Arizona of a conference on THE GALAXY AND THE SOLAR SYSTEM. The conference resulted in a book in the Space Science Series of the University of Arizona press. Similarly, our interest in solar system ices led to a NATO-sponsored 1984 conference in Nice, France on THE ICES IN THE SOLAR SYSTEM which resulted in a book under the same title. 10P

### 1. ICES

#### a) Structure of Ices on the Jovian and Saturnian Satellites and on Planetary Rings

A critical analysis has been made of the nature and structure of H<sub>2</sub>O- and other ices on satellites of the outer planets. This study was based on the results of our earlier investigations of the effect of meteoritic bombardment, pressure densification and pore diffusion in a thermal gradient in porous ices. The basic questions which at that time were unanswered pertained to the role of purity of ices, the values of the initial and equilibrium porosity as well as the magnitude of the thermal gradients. These quantities may vary significantly from one site to another. Making reasonable assumptions one concludes that the icy surfaces are mostly crystalline and partly amorphous and that the fraction of amorphous ice should be lower in the Saturnian than Jovian system. It should be also lower for smaller than for larger satellites. On large, partly icy satellites such as Ganymede and Callisto, the high pressures may have led to closing of pores in parts of their icy interiors. The meteoritic bombardment and pore diffusion would produce thin dense surface layers on these two satellites which should thus show high thermal inertia. If Enceladus and Europa indeed have internal heat sources produced by tidal effects, as has often been suggested, their surface would tend to be more porous than the deeper layers and this would improve thermal insulation and lower the thermal inertia of their surfaces. These conclusions may be observationally verifiable.

The small size of the icy particles in the Saturnian rings and the strong meteoritic and proton bombardments of the particles in these rings lead to conclusions which differ from those for icy satellites described above. Here the continuous processes of resurfacing, collisions, break-up and aggregation result in a relatively short-lived exposure of a particular area of crystalline or amorphous ices to the environment, in the presence of negligible thermal gradients, in high brightness, in low mechanical strength and in low thermal inertia.

#### b) Cometary Nuclei

The influence of porosity and degree of crystallinity on the structure, heat transport and heat balance in cometary nuclei has been extensively studied. The observed behavior

of a comet is dominated by the heat transport in the nucleus which can be understood in terms of the large scale structure, such as shape and inhomogeneity, and the thermal properties of the fine structure, porous, icy materials that compose the nucleus. Results focus on the role of the small scale structure, such as pore shape and size, in the evaluation of effective thermal conductivities for comet material. Three dimensional finite element models have been developed to calculate the effective thermal conductivity of crystalline and amorphous water ices as a function of porosity pore shape, pore size, pore vapor composition, pore orientation with respect to heat flow, pore size distribution, pore packing geometry, and grain-grain interface size. The modeling has included heat transport due to solid and vapor conduction, viscous and Knudsen flow, and radiation across the pore space. As well as serving as the input for calculations of the large scale heat transport, the fine scale results offer insight into the influence of pores on the transport of heat in comet material. Arguments, based on laboratory measurements of condensation products and the mechanics and evolution of porous icy materials, agree with larger estimates for comet density. In particular, calculations indicate that the thermal stress within a comet near perihelion would exceed the fracture strength of a highly porous, low density comet matrix material. The fact that relatively few comets are observed to fracture catastrophically lends support to the hypothesis favoring a higher density comet material such as that recently proposed by S. Peale. Given this evidence in support of a higher density, lower porosity materials, the calculations focus on determining the effective thermal conductivity of a higher density, lower porosity icy comet matrix.

The thermal conductivity of non-porous water ice is a strong function of temperature. Calculations of the effective thermal conductivity of water ice include the contribution of the pore space to the conductivity of the material. At low temperatures, the pore space impedes the flow of heat in the material, thus lowering the effective conductivity. At temperatures above  $\sim 200$  K, water vapor in the pore space can greatly enhance the effective thermal conductivity. For example, in non-porous water ice at 80 K and 24 K, the thermal conductivities are  $7.1 \text{ Wm}^{-2}\text{K}^{-1}$  and  $2.4 \text{ Wm}^{-2}\text{K}^{-1}$ . At 25% porosity, with spherical  $1 \text{ mm}$  pores, the corresponding thermal conductivities are  $4.7 \text{ WM}^{-2}\text{K}^{-1}$  and  $3.6 \text{ WM}^{-2}\text{K}^{-1}$ , not including the contribution from the radiative heat transport. At low temperatures, the thermal conductivity is decreased by 33% due to the influence of the virtually empty pore space. The empty pores space is ineffective at conducting heat through the material. However, at high temperatures, the pore space vapor causes the effective thermal conductivity to increase by 53% again apart from radiative heat flow. In another part of this study, the influence of pore shapes on the effective thermal conductivity was investigated. As an example of the potentially great influence of pore shape, for a 25% porous water ice material with ellipsoidal, cigar shaped  $1 \text{ mm}$  pores, the effective thermal conductivities were calculated to be  $5.2 \text{ Wm}^{-2}\text{K}^{-1}$  and  $4.4 \text{ Wm}^{-2}\text{K}^{-1}$  at 80 K and 240 K. Similarly, for a thin, pancake shaped pore of the same volume, the effective thermal conductivities were  $1.7 \text{ WM}^{-2}\text{K}^{-1}$  and  $3.5 \text{ Wm}^{-2}\text{K}^{-1}$  at the corresponding temperatures. The material possessing the long, cigar shaped pores is extremely effective at transporting heat at the high temperatures. The thermal conductivity is increased by 21% over that of the material containing spherical pores. This is in contrast to the conductivity of the material containing pancake shaped pores in which the conductivity was only 2% above the value for the material possessing the spherical pores. Due to their orientation with respect to the flow of heat, the flat pancake shaped pores do not act as efficient channel for heat flow as do the long, cigar shaped pores. Similar comparisons can be made for low temperatures, in which we see that the pancake shaped pores cause a greater reduction in the effective thermal conductivity than do the cigar shaped pores, a 63% reduction versus a

9% reduction. The pancake shaped pores greatly impede the flow of heat through the material. These are just two examples out of the many cases that have been calculated in this study. As stated above, the effect of porosity, pore shape, pores size, pore orientation, pore size distribution, pore vapor composition, solid ice composition, grain/pore packing, grain-grain interface relative dimension and transport mechanism were included in this research.

It has been shown that since, in a thermal gradient, porous CO<sub>2</sub>-ice densifies much faster than H<sub>2</sub>O-ice, the heat content of the interiors of CO<sub>2</sub>-rich cometary nuclei will be higher than in nuclei which are H<sub>2</sub>O-rich. As a result, the former will tend to break up when the CO<sub>2</sub>-gas pressure in the interior becomes locally high; on the other hand, H<sub>2</sub>O-ice rich nuclei may show only brightness outbursts. It follows from the analysis that both of these phenomena: splittings and outburst should occur preferentially after rather than before, the perihelia. This conclusion is in agreement with H. Campins statistical analysis of cometary observations.

Considerable progress has been made in modeling the role of the dust content and porosity of icy cometary nuclei. The influence of differential thermal expansion of the constituents on the coherency of the nuclei has been analyzed with the result that if, in the pertinent range of temperatures, the non-icy constituents form a sufficiently large coherent area they will break away from the surrounding ice especially if the latter is amorphous. Also, the thermal diffusivity of dust-ice mixtures with various porosities has been determined. It appears that depending upon composition and porosity the thermal conductivity of cometary ice can vary by orders of magnitude in temperature range between 20K and 250K. At low temperatures, the pores decrease the thermal conductivity of ice while at higher temperatures they increase it, by contributing the rapid heat flow through vapor-filled pores. In porous crystalline ice, the effective thermal conductivity has a deep minimum around 100K while in amorphous porous ice the conductivity increases rapidly until the crystallization temperature and then, depending on porosity and nature of the volatiles it either increases or decreases with temperature.

The effect of the variation of thermal conductivity with temperature on the radial temperature profile of cometary nuclei has been numerically evaluated. The influence of these changes on the surface temperature of an isothermal nucleus and on the ensuing brightness of the comet's coma has been analyzed making it possible for the first time to deduce the effective thermal conductivity of the nuclei of various comets from observational data. Subsequently, making plausible assumptions about the size of pores size one can estimate the apparent porosity of the comets. The results are as follows: P/KOFF 0.3, P/HALLEY 0.2, P/d'ARREST 0.4, P/GIACOBINI-ZINNER 0.5 AND P/ENCKE 0.1. Interestingly enough, P/KOPFF shows a progressive drop of porosity, that is, a densification of its nucleus over the last 60 years. It should be stressed that because of the various simplifying assumptions the thus calculated porosities should be taken as having primarily a relative and not absolute significance.

### c) Mechanical Properties of Cometary Nuclei

So far, only a few studies have been made of the mechanical behavior of cometary nuclei in spite of its importance for quantitative understanding of sudden flare-ups and splittings. As an initial step the basic Griffith-type theory of fracture has been applied by J.R. Green to a homogeneous, polycrystalline, all H<sub>2</sub>O-ice, nucleus. The critical length of Griffith cracks varies from one to a few hundred microns depending on surface

temperature. In general, tangential hoop stresses turn out to be more important than the radial stresses but their variation with temperature is not monotonic.

## II. CLATHRATES

There is a fairly wide consensus that the appearance of certain highly volatile species in cometary spectra indicates the presence of clathrates in cometary nuclei. The mechanism of their formation, growth and of their subsequent dissociation has, so far, not been investigated. One of the most important is the CO<sub>2</sub>-clathrate, which exists only above about 120 K and below the melting point. Density changes accompanying CO<sub>2</sub>-clathrate formation and decomposition lead to microporosity and thus enhanced brittleness or even to fracture of cometary nuclei at low temperatures. In order to understand quantitatively the mechanism of its formation and dissociation at low temperatures, the energy of motion of a CO<sub>2</sub> molecule from its position in a large cage through a hexagonal face common to two adjoining large cages in the clathrate lattice has been quantum-mechanically calculated using the Hartree-Fock theory (with J.S. Binkley). On this model the energy of activation for motion of the linear CO<sub>2</sub> molecule through a rigid, i.e., unrelaxed, clathrate lattice turns out to be about 0.27 eV. In the next step, the neighboring atoms of the lattice relax which lowers this energy in agreement with the value of 0.05 to 0.10 eV estimated on the basis of the experimental data of D.W. Davidson.

## III. THE BOUNDARY OF THE SOLAR SYSTEM AND THE OORT CLOUD

The shape of the boundary of the solar system defined as the surface within which the Sun, rather than the rest of the galaxy, controls the motion of bodies such as comets, has been determined by taking into account the perturbations of extended orbits by the gravitational field of the galactic center and of the galactic mid-plane. It appears that the limiting orbits are non-Keplerian and those which are prograde have different limits than retrograde orbits. Besides, neither boundary is a simple sphere and both boundaries are much larger than the usually assumed size of the Oort cloud.

The possibility that the presumed periodic cometary/asteroidal showers and the associated biological extinctions could be explained without an ad hoc assumption of the existence of a solar companion star NEMESIS or of planet X has been investigated. The paths of 12,000 cometary bodies have been followed to assess the effect of the known slightly anharmonic galactic z-potential in the direction perpendicular to the galactic plane. The effect turns out to be positive though very small and further study is required. No further work along these lines has been done.

## IV. INTERSTELLAR DIFFUSE ABSORPTION LINES

We have been successful in accounting for the order of magnitude of the width of the interstellar diffuse absorption lines produced by atoms entrapped in thin graphitic shells C<sub>60</sub> in terms of the change of the volume available to the excited electron. Also, the existence of a number of pairs of absorption lines can be understood if free vibrations of the thin shells are taken into account. A study has been made of the possible mechanisms and sites in space where the carbon shells C<sub>60</sub> could be formed. The most efficient sites appear to be the SNI supernovae. It is hoped that this model explains the intensity and the total number of the interstellar diffuse absorption lines in terms of known atomic spectra.

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June, 1990

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